1. Introduction

Most of the CFD analysis of flow problems in complex configurations in general use finite-difference, finite volume or finite element methods for numerical solution of a system of strongly coupled non-linear partial differential equations relevant to the convective diffusive transport processes of fluid mechanics. The accuracy of any solution algorithm depends to a large extent on the discretisation schemes used for numerical simulation of the differential operators in the relevant equations which often involve both temporal (with respect to time) and spatial (with respect to the coordinate directions in space) derivatives. Since most of the CFD algorithms use the concept of time-marching in numerical solution, the temporal derivatives are almost always replaced directly by their discretised analog. In case of spatial derivatives however, how the discretisation scheme enters the solution procedure depends on whether it is a finite difference or a finite volume (or element) procedure. In finite difference methods, the discretisation schemes straightaway replace the partial derivatives by the equivalent discretised form. On the other hand, in finite volume methods, when the differential equations are integrated over a finite control volume, the discretisation scheme, in principle, decides the internodal variation of the flow variables along the different spatial direction. In other words in the integral form of the conservation equations, the spatial discretisation schemes behave more like an interpolation procedure to evaluate the variable value or its gradients at any point in the field using the nodal values surrounding the point in question. The order of accuracy is conventionally denoted in the sense of a Taylor series expansion of the relevant derivative which, in the discretised form, is always truncated up to certain terms only. The problem is even more serious in case of RANS codes for computation of turbulent flow where the errors may consist of discretisation error as well as the errors arising out of the approximations in the turbulence model. Any reasonable assessment of the performance of a turbulence model is almost impossible unless the code developer has full control on the level of accuracy and errors from the discretisation schemes used. LES (Large Eddy Simulation) and DNS(Direct Numerical Simulation) calculations are aimed at understanding more about the physics and mechanism of turbulent flow through time-accurate calculation of three-dimensional flow. Obviously in such cases large discretisation errors may lead to absolutely wrong explanation of a time- and space-dependent physical phenomenon. Analysis and study of discretisation schemes therefore form a very important step in the development of any CFD algorithm for analysis of problems with variety of geometrical and physical complexities.

1.1 Scope of the present work

The present work describes the algebra involved in the two temporal and four different spatial discretisation schemes used in the existing pressure-based code RANS3D developed in the CTFD Division, NAL during the last ten years [4-7]. Two simple problems have been chosen to assess the accuracy of these different discretisation schemes in analysing flow problems involving convective and diffusive transport processes. The first problem computes the purely convective transport of a passive scalar profile in the form of a rectangular and a sinusoidal form in a uniform one dimensional flow and the second problem computes the viscous decay of a two-dimensional vortex for which the analytical Taylor's solution is available for comparison.

Chapter 2 discusses the different discretisation schemes and the results obtained for the two test flow situations are discussed in chapter 3. Some concluding remarks are given in chapter 4.

2. Numerical discretisation schemes

The generalised form of the scalar transport equation for laminar incompressible (density is therefore taken out of the equation) flow may be written in tensor form as following where '*i*' is a summing index:

$$\frac{\partial\phi}{\partial t} = -\frac{\partial}{\partial x_i}(u_i\phi) + \frac{\partial}{\partial x_i}\left(D\frac{\partial\phi}{\partial x_i}\right) + S_\phi \qquad (2.1)$$

where the left hand side is the time-dependent unsteady term and the three terms on the right hand side are the convective, diffusive and the source terms respectively which involve the spatial gradients of the scalar as well as those of the velocity components and D is a generalised diffusion coefficient. This equation can be considered to be of a generic form since if ϕ is replaced by the velocity components u_i, D represents the fluid viscosity and the source terms are replaced by the pressure gradient term, the above equation only represents the conservation of momentum components. Further for mass conservation, the velocity field needs to satisfy the continuity equation as

$$div\,V = \frac{\partial\phi}{\partial x_i} = 0 \qquad (2.2)$$

The left hand side of the Eq. 2.1 deals with the temporal discretisation and the convective and diffusive fluxes involving the spatial discretisation appear in the right hand side. The diffusive terms being linear in ϕ can always be discretised accurately under the assumption of linear internodal variation of the flow variables. But the overall success of the solution algorithm is decided by how the non-linear convective terms are discretised. Various discretisation schemes formulated and implemented in the RANS3D algorithm are described in the next two subsections.

2.1 Temporal discretisation schemes

2.1.1 Two Level Euler Backward scheme

Any physical process is parabolic in time and the time derivative of ϕ appearing in the left hand side of the Eq. (2.1) can always be expressed in an Euler backward difference form as following:

$$\frac{\partial\phi}{\partial t} = \frac{\phi^{(n+1)} - \phi^n}{\Delta t} \qquad (2.3)$$

where $\phi^{(n+1)}$ and ϕ^n are the values of ϕ at $(n+1)^{th}$ and n^{th} time steps and Δt = size of the timestep = $t^{(n+1)} - t^n$ Replacing $\frac{\partial\phi}{\partial t}$ in Eq. 2.1 one obtains

$$\phi^{(n+1)} = \phi^n + \Delta t\,(R) \qquad (2.4)$$

where R is the discretised value of the right hand side of equation (Eq. 2.1) and function of ϕ, velocity components and their gradients. In case of the so-called explicit schemes, R is evaluated at the old time level (t^n) and hence the calculation advances in time to compute $\phi^{(n+1)}$ explicitly. But in implicit solution procedure the velocity and the field of ϕ in the right hand side is assumed to be at the unknown $(n+1)^{th}$ level and hence a system of linear equations needs to be solved. In the present finite volume implicit scheme employed in RANS3D algorithm both R and the left hand side time derivatives are expressed in integral form in the so-called flux balance equation as follows

$$R^{(n+1)} = A_W(\phi_W - \phi_P) + A_E(\phi_E - \phi_P) + A_S(\phi_S - \phi_P) + A_N(\phi_N - \phi_P) + A_B(\phi_B - \phi_P) + A_T(\phi_T - \phi_P) + \mathrm{SU} \quad (2.5)$$

$$\text{and } \phi^{(n+1)}\frac{\Delta v}{\Delta t} = R^{(n+1)} + \phi^n \frac{\Delta v}{\Delta t} \quad (2.6)$$

where Δv is the volume of the cell and Δt is the size of the time step.

Replacing $R^{(n+1)}$ from Eq. 2.5, one obtains the final system of linearised equations to be solved as the following :

$$\left(A_P + \frac{\Delta v}{\Delta t}\right)\phi^{(n+1)} = \sum_i A_i\phi_i + SU + \phi^n \frac{\Delta v}{\Delta t} \quad (2.7)$$
$$\text{for } i = W, E, S, N, B, T \text{ and } A_P = \sum_i A_i$$

where ‘i’ indicates the six neighbouring locations (west, east, south, north, bottom and top) of the cell centre P in question.

The coefficients A_i however, are functions of velocity components and the solution at each time step therefore needs iterative procedure to be followed for accurate solution of the coupled non-linear system. This scheme is known to be first order accurate in time and significant error may occur in some problems even with reasonable time step size and choice of excessively small time step for accurate solution often enhances the computation time to a prohibitive level.

2.1.2 Three Level Fully Implicit scheme

This scheme, claimed to be second order accurate in time, assumes a quadratic variation of the variable ϕ at three consecutive time instants. Accordingly the first derivative of the variable ϕ with respect to time at the $(n+1)^{th}$ level may be written as following:

$$\frac{\partial\phi}{\partial t} = \frac{1.5\phi^{(n+1)} + 0.5\phi^{(n-1)} - 2\phi^n}{\Delta t} \quad (2.8)$$

Equating the right hand side expression to the left hand side of the implicit flux balance equation (Eq. 2.4) one obtains,

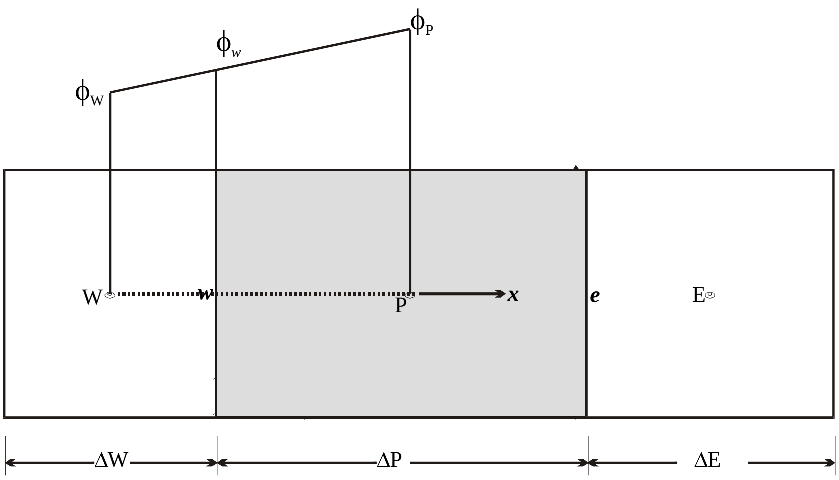
$$\left(A_P + 1.5\frac{\Delta v}{\Delta t}\right)\phi^{(n+1)} = \sum_i A_i\phi_i + SU + 2\phi^n \frac{\Delta v}{\Delta t} - 0.5\phi^{(n-1)} \frac{\Delta v}{\Delta t} \tag{2.9}$$

$$\text{for } i = W, E, S, N, B, T \text{ and } A_P = \sum_i A_i$$

2.2 Spatial discretisation schemes

The right hand side of Eq.2.9 consists of the convective and diffusive terms containing spatial derivatives of ϕ and the velocity components. In the finite volume form these spatial derivatives are transformed to fluxes across the cell faces and the discretisation scheme basically decides the interpolation to be used for evaluation of cell face value of the variable or its gradients from the nodal values at either side of the face. The schemes are described here schematically in a 1D flow situation and the principle can be easily extended separately along three coordinate directions for a 3D situation. The diffusive fluxes can always be discretised using a linear internodal variation of the different flow variables. But the discretisation of the convective fluxes involving the flow variable values and mass fluxes at the cell face is the most critical step in order to achieve successful numerical convergence of the scheme. The major issue is how to evaluate the value of a flow variable at any cell face lying between two consecutive cell centres. Four different flux discretisation schemes used in the present finite volume procedure RANS3D are given here below.

2.2.1 Central Difference scheme



Typical 1D control volumes

Fig 2.1 Schematic sketch for Central Difference scheme

This scheme assumes a linear variation between the values of the variable at the cell centres *W* and *P* lying upstream and downstream of a cell face *w* and hence computes the value at the cell face *w* as

$$\phi_w = f_P\phi_P + (1 - f_P)\phi_W \tag{2.10}$$

where $f_P = \Delta W / (\Delta P + \Delta W)$ and ΔW and ΔP represent the size of the cell with centres at *W* and *P* respectively. Now based on the assumption of linear internodal variation, the total flux at the face *w* may be written as :

$$\text{Flux at } w = C_w\phi_w + D_w(\phi_P - \phi_W) \tag{2.11}$$

Replacing ϕ_w from Eq. 2.10 and using the same linear variation for the east face *e*, one obtains the final flux balance equation for the cell as following:

$$A_P\phi_P = A_W\phi_W + A_E\phi_E + SU \tag{2.12}$$

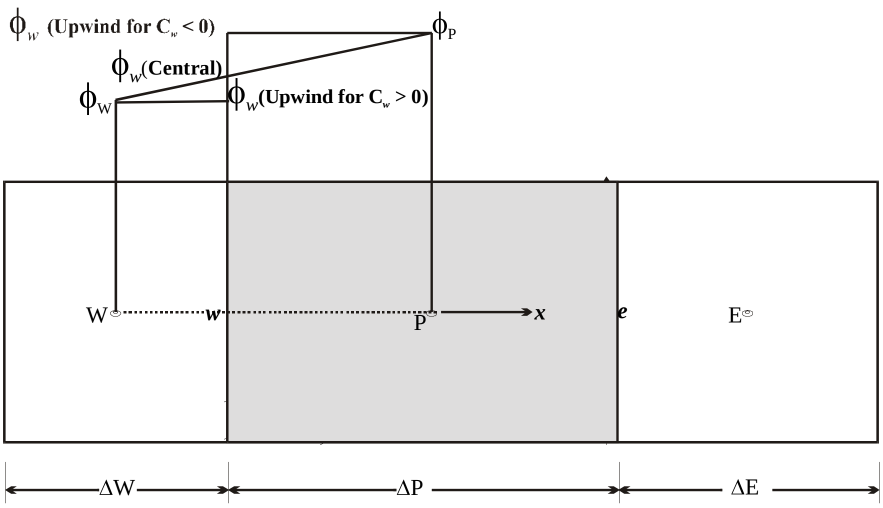
where

$$A_W = D_w + C_w(1 - f_P)$$
$$A_E = D_e - C_e f_E$$

C_w and C_e are convective mass fluxes and D_w and D_e are diffusion coefficients at the faces *w* and *e* respectively and $f_E = \Delta P/(\Delta P + \Delta E)$.

When the flow velocities and hence the convective fluxes are very small compared to the diffusive fluxes (convective is less than the half of the diffusive flux) at any cell face, the central difference scheme is numerically stable. But direct use of the above coefficients for high Reynolds number flow often lead to non physical oscillations or wiggles for the flow variables in the solution; sometimes the amplitude of the oscillations may even be quite large causing numerical divergence. Such failure of the numerical process may often be attributed to the generation of large negative coefficients (A_W or A_E) of the linear equation system. For such numerical instabilities, the Deferred Correction procedure [1] described in the next section, is recommended to be a good solution which uses a weighted mixing of the fluxes derived from two different schemes.

2.2.2 Central / Upwind Hybrid Scheme



Typical 1D control volumes
Fig 2.2 Schematic sketch for Central/Upwind Hybrid scheme

This is a composite scheme [9] which assumes a pure Upwind interpolation for the face value of the variable if the grid Peclet number is more than 2 and otherwise a Central Difference interpolation assuming linear variation between the values of the variable at the cell centres *W* and *P* lying upstream and downstream of a cell face *w*. The Upwind interpolation takes care of the direction of the velocity signal propagation and assumes the variable value at the face to be the same as the value at the immediate upstream node.

$$\begin{aligned} \phi_w &= \phi_W \text{ if flow is from } W \text{ to } P\ (C_w > 0) \\ &= \phi_P \text{ if flow is from P to W } (C_w < 0) \end{aligned} \tag{2.13}$$

The Peclet number is defined as the ratio of the convective and the diffusive coefficients at any cell face. The variable value at the cell face ϕ according to Central/Upwind hybrid difference scheme may be written as:

$$\phi_w = f_P \phi_P + (1 - f_P)\phi_W \tag{2.14}$$

where

$$f_P = \Delta W / (\Delta P + \Delta W) \quad \text{if} \quad Pe \ \ (= C_w / D_w) \le 2 \ \ \text{(Central)}$$

$$f_p = 0.5\left[\left(C_w + |C_w|\right)/C_w\right] \quad \text{if} \quad Pe \ \ (= C_w / D_w) > 2 \ \ \text{(Upwind)}$$

Where ΔW and ΔP represent the size of the cell with centres at W and P respectively. Using such composite interpolation for the cell-face variable values, required in the convective flux evaluation , the final flux balance equation for a 1D control volume can be written in the following form.

$$A_P \phi_P = A_W \phi_W + A_E \phi_E + SU \tag{2.15}$$

where

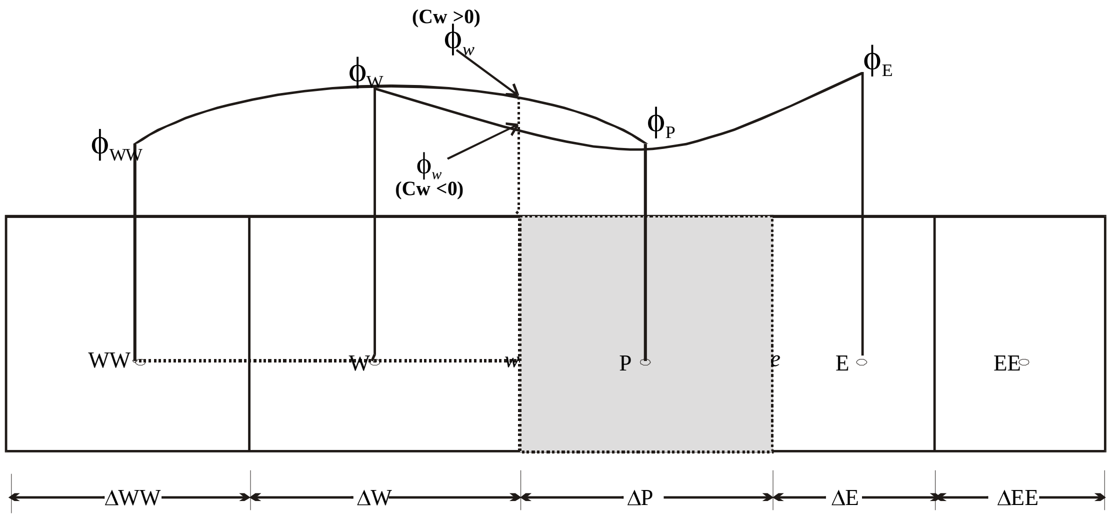
$$\begin{aligned} A_W &= D_w . Max(0.,1 - 0.5|C_w / D_w|) + Max(0.,C_w) \\ A_E &= D_e . Max(0.,1 - 0.5|C_e / D_e|) + Max(0.,-C_e) \end{aligned}$$

and *Max* function denotes the maximum between the two arguments of the function.

The Upwind procedure is well known [8] to ensure numerical convergence through damping of the numerical instabilities; but at the same time the scheme also yields large numerical diffusion deteriorating the numerical accuracy of the solution, specially when the flow is skewed to the grid lines. The numerical diffusion errors reduce as the grid size reduces and basically in the Hybrid scheme when the grid size is small, the grid Peclet number is low and, if less than 2, the scheme switches to Central difference which is second order accurate with less numerical diffusion and less of instability problem as well.

2.2.3 QUICK(Quadratic Upwind Interpolation for Convection Kinematics) Scheme

The QUICK scheme was first proposed by Leonard [2] as a third order accurate scheme with numerical diffusion reduced to minimum. This scheme assumes a Quadratic Upwind interpolation for the face value of the variable by assuming a second order polynomial (parabola) through the downstream, upstream and one node further upstream nodes of the cell face in question. In case $C_w > 0$ *i.e.*, the flow is from *W* to *P*, the node *W* is the upstream, *P* is the downstream and *WW* is the further upstream node for the face *w*. For $C_w < 0$ *ie.*, the flow is from *P* to *W* the node *P* is the



Typical 1D control volumes

Fig 2.3 Schematic sketch for QUICK scheme

upstream, *W* is the downstream and *E* is the further upstream node for the face *w*. The variable value ϕ_w at the cell face *w* according to a quadratic interpolation between ϕ_P, ϕ_W, ϕ_{WW} for $Cw > 0$ may be written as:

$$\phi_w = \phi_W + Ax^2 + Bx \tag{2.16}$$

where $x = 0.5\,\Delta_W$ and the origin is assumed to lie at the node *W*. Satisfying the nodal values of ϕ at *P*, *W* and *WW*, the values of the coefficients *A* and *B* may be determined as :

$$\begin{aligned} A &= 4(QR + PS)\big/(P^2Q + PQ^2) \\ B &= 2(Q^2R - P^2S)\big/(P^2Q + PQ^2) \end{aligned} \tag{2.17}$$

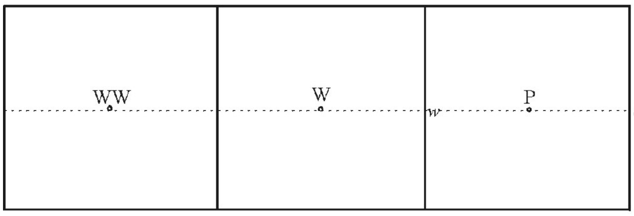
where $P = \Delta_P + \Delta_W$, $Q = \Delta_W + \Delta_{WW}$, $R = \phi_P - \phi_W$ and $S = \phi_{WW} - \phi_W$ and Δ_P, Δ_W and Δ_{WW} represent the size of the cell with centers at *P*, *W* and *WW*.

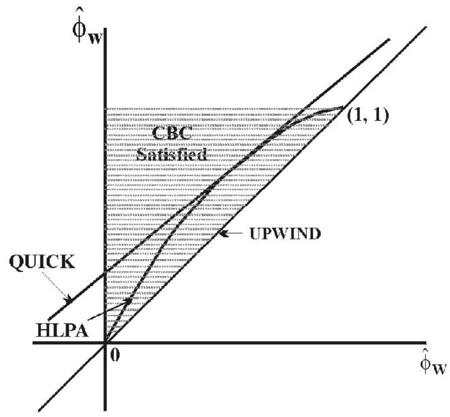
Using quadratic upwind interpolation for evaluation of the cell-face variable values, as described above, the final flux balance equation for a 1D control volume can be written in the following form.

$$A_P\phi_P = A_W\phi_W + A_E\phi_E + A_{WW}\phi_{WW} + A_{EE}\phi_{EE} + SU \tag{2.18}$$

But quadratic interpolations are often not guaranteed for the boundedness property. The interpolants may in some cases have values which are larger than the maximum value of the data at the three input nodes. This may lead to oscillatory solutions with under or overshoots beyond the realistic values of the physical variables. The numerical instability problem, if any, can be avoided using the deferred correction procedure described in the next section.

2.2.4 HLPA (Hybrid Linear Parabolic Approximation) scheme





(a) Typical control volume and related nodes **(b) Normalised variable diagram**

Fig 2.4 Different Upwind schemes on a normalised variable diagram

The HLPA scheme, first proposed by Zhu [10], is basically a compromise between the large numerical diffusion of the 1st order upwind schemes and the numerical instability problem for the accurate higher order upwind schemes with low numerical diffusion. The principle used is based on the so-called Convection Boundedness Criterion (CBC) of such convective flux schemes first reported by Gaskell and Lau [3] which is briefly discussed below.

If the west face *w* of the control volume shown in fig.2.4(a) is considered and it is further assumed without loss of generality that the flow is from W to P (*i.e.*, $C_w>0$), the scalar variable ϕ may be normalised in an upwind biased sense as :

$$\hat{\phi} = (\phi - \phi_{WW})/(\phi_P - \phi_{WW}) \tag{2.19}$$

Assuming the existence of a continuous increasing function or union of piecewise continuous increasing function that relate the normalized face value to the normalized upstream value $\hat{\phi}_W$, *i.e.*, $\hat{\phi}_w = f(\hat{\phi}_W)$, Gaskell and Lau [3] formulated the Convection Boundedness Criterion (CBC) as follows. A numerical approximation to $\hat{\phi}_w$ is bounded if

(i) for $0 \le \hat{\phi}_W \ge 1$, f is bounded below by the function $\hat{\phi}_w = \hat{\phi}_W$ and above by unity and passes through the points (0,0) and (1,1)

(ii) for $\hat{\phi}_W < 0$ or $\hat{\phi}_W > 1$, f is equal to $\hat{\phi}_W$

The first condition physically signifies that if $\phi_{WW}<\phi_W<\phi_P$ the function is increasing in a monotonic manner and then the condition $\phi_W<\phi_w<\phi_P$, satisfied by any interpolation scheme will ensure boundedness. On the other hand if $\phi_W < \phi_{WW}$ or $\phi_W>\phi_P$, ϕ_w is simply taken to be ϕ_W as per the pure upwind formulation since then the monotonicity of the function is not preserved in the interval between *P* and *WW* in which the quadratic interpolation is intended to be used. The quadratic interpolant then has either a maxima or a minima at the node *W*.

The CBC is illustrated in fig 2.4(b) where $\hat{\phi}_w = \hat{\phi}_W$ and the shaded triangular area is the region over which the CBC is valid and in the range $\hat{\phi}_w < 0$ or $\hat{\phi}_w > 1$, it follows the 45^o line indicating $\hat{\phi}_w = \hat{\phi}_W$ everywhere. The importance of CBC is to provide a sufficient and necessary condition for guaranteeing the bounded solution if at most three neighbouring nodal values are used to approximate the face values. It is known that the sufficient condition for boundedness is that the coefficients of the finite difference equation should be positive, but the existence of negative coefficients does not necessarily lead to over- or undershoots.

In the normalized form for equally spaced grids ($\Delta_P = \Delta_W = \Delta_{WW}$ in Fig. 2.3), the QUICK scheme interpolates ϕ_w as following

$$\hat{\phi}_w = 0.75\hat{\phi}_W + 3.75 \tag{2.20}$$

where the pure upwind scheme may be expressed as

$$\hat{\phi}_w = \hat{\phi}_W \tag{2.21}$$

These two different linear characteristics are shown in fig 2.4(b) and it is clearly observed that the pure upwind scheme can unconditionally satisfy the CBC. The Hybrid Linear Parabolic Approximation (HLPA) scheme basically assumes a quadratic (Parabolic) variation of $\hat{\phi}_w$ only in the monotonic range ($0 < \hat{\phi}_W < 1$) when it deviates from the pure upwind scheme and lies close to QUICK. When the variation of $\hat{\phi}_w$ is not monotonic, $\hat{\phi}_w$ varies with $\hat{\phi}_W$ in a linear manner with unit slope, representing first order accurate pure Upwind scheme. In the normalized form, the HLPA scheme is defined as follows:

$$\hat{\phi}_w = \begin{cases} \hat{\phi}_W\left(2 - \hat{\phi}_W\right) & \text{if } 0 < \hat{\phi}_W < 1 \\ \hat{\phi}_W & \text{otherwise} \end{cases} \tag{2.22}$$

This non-linear characteristics of HLPA scheme is represented in Fig.2.4(b). In case $C_w > 0$ *i.e.*, the flow is from *W* to *P*, the node *W* is the upstream, *P* is the downstream and *WW* is the further upstream node for the face *w*. For $C_w < 0$ *ie.*, the flow is from *P* to *W* the node *P* is the upstream, *W* is the downstream and *E* is the further upstream node for the face *w*. It is to be noted that QUICK assumes a quadratic variation of the variable ϕ itself along the grid line but means a linear variation of the non-dimensional variable $\hat{\phi}_w$ as shown in Fig. 2.4(b) whereas the HLPA assumes a quadratic variation of the variable $\hat{\phi}_w$ itself as shown in the same figure. It is also interesting to note how QUICK satisfies the CBC only in a limited range of $\hat{\phi}_w$. For values of $\hat{\phi}_w$ lying outside the shaded region QUICK may yield unbounded solution although numerical diffusion is reduced to minimum. The variable value ϕ_w at the cell face w according to the HLPA scheme between ϕ_P, ϕ_W, ϕ_{WW} for $Cw > 0$ in terms the non-normalized variable may be rewritten as following which represents a second order accurate upstream weighted approximation of the value of ϕ at the face w:

$$\phi_w = \phi_W + \gamma(\phi_P - \phi_W)\hat{\phi}_W \tag{2.23}$$

$$\text{where } \gamma = \begin{cases} 1 \ \text{ if } \ \left|\hat{\phi}_W - 0.5\right| < 0.5 \\ 0 \ \text{ otherwise} \end{cases}$$

$$\text{and } \hat{\phi}_W = (\phi_W - \phi_{WW})/(\phi_P - \phi_{WW})$$

Using this composite second order accurate upwind interpolation scheme for evaluation of the cell-face variable values, the final flux balance equation for a 1D control volume can be written in the following form where the coefficients A however are different from those of the QUICK scheme.

$$A_P\phi_P = A_W\phi_W + A_E\phi_E + A_{WW}\phi_{WW} + A_{EE}\phi_{EE} + SU \tag{2.24}$$

2.3 Deferred correction procedure for the flux balance equation

In this procedure, a suitable weighting function is used to blend the flux from the desired scheme with upwind fluxes which allows some small numerical diffusion and ensures numerical stability of the solution. The flux balance equation using pure upwind scheme for 1D control volume may be written as:

$$A_{PU}\phi_P = A_{WU}\phi_W + A_{EU}\phi_E + SU \tag{2.25}$$

For any other general scheme used, the same balance equation may be written as:

$$A_P\phi_P = A_W\phi_W + A_E\phi_E + SU \tag{2.26}$$

Eq. 2.25 can now be rearranged as following

$$A_{PU}\phi_P = A_{WU}\phi_W + A_{EU}\phi_E + SU + \alpha_U \ SUH \tag{2.27}$$

where $SUH = \phi_E(A_E - A_{EU}) + \phi_W(A_W - A_{WU}) - \phi_P(A_P - A_{PU})$. And α_U is the deferred correction factor ranging between 0 and 1. α =0 represents pure upwind flux and α_U =1 represents the flux as per the desired scheme. The value of this factor α may even be varied from a low value in the beginning of the iteration sweep to a larger value towards the end of the convergence process allowing minimum numerical diffusion and hence more accurate results. Irrespective of the scheme used, the coefficients of the linear equation system are always retained to be positive according to upwind formulation whereas the difference between the actual fluxes and the upwind fluxes are added to the balance equation to the source terms *SUH*. In case of multi-dimensional flow the same one-dimensional principle described above is used independently along all the directions.

3. Results and discussions

This section discusses the results obtained for two test problems to assess the accuracy of the RANS3D algorithm employing different combination of the temporal and spatial discretisation schemes described above.

3.1 Pure convective transport of a scalar profile

This test problem has been chosen to examine the performance of the discretisation schemes in resolving a sharp spatial gradient of a passive scalar variable ϕ in a uniform 1D flow. At $t=0$, a rectangular or a sinusoidal profile of a scalar is placed at a certain location of the flow and tracked how the profile advances in time with the given inviscid uniform flow. Analytically in absence of any physical viscosity, the profile should simply be transported along the flow without any distortion. Any deviation from this ideal situation may be attributed to the numerical diffusion arising out of the truncation error of the discretisation schemes used.

The computational domain consists of a rectangular 2D space of unit width covering 100 units of length. A uniform grid with $\Delta x = 0.2$ is used (500 control volumes in x-direction and 1 control volume in the y-direction) and the viscosity is set to an insignificant small value ($1\text{x}10^{-20}$). The scalar transport equation is only solved with prescribed uniform velocity of unity along the x-direction. The time step size Δt is chosen as 0.1. The scalar profile of unit amplitude is prescribed either in a rectangular or a sinusoidal form between $30 < x < 50$ and zero elsewhere. At the outflow plane the streamwise gradient of ϕ is set to zero. On the top and bottom boundary of the computation domain, symmetry condition (*i.e*. normal gradient of ϕ is set to zero) were used to ensure one-dimensional flow. All the four spatial discretisation and the two temporal discretisation schemes have been used for numerical solution of the problem and the results are shown in Figs. 3.1 to 3.4.

Fig. 3.1 shows the effect of the discretisation scheme on the transport of the rectangular profile of a scalar quantity after t=100 units using the 1st order accurate temporal scheme and the following observations are made:

- For the Central/Upwind HYBRID Scheme (which is basically pure upwind in the present case since diffusion is zero), the rectangular profile after t=100 is diffused to form a Gaussian distribution with a large lateral dispersion where the amplitude is reduced to almost 93% of the input peak of unity.
- For HLPA, QUICK and CD Scheme the rectangular profile even after the elapse of 100 units of time is smeared with a very small lateral spread along the x-direction and the amplitude of $\phi=1$ is maintained for some distance in the beginning. The very slow decay of the peak amplitude and the small smearing of the profile in the sharp gradient zone, demonstrate the small numerical diffusion of these schemes. Some overshoot and undershoot are observed only in the initial time steps when QUICK or CD schemes are used, which disappear by the instant t=100

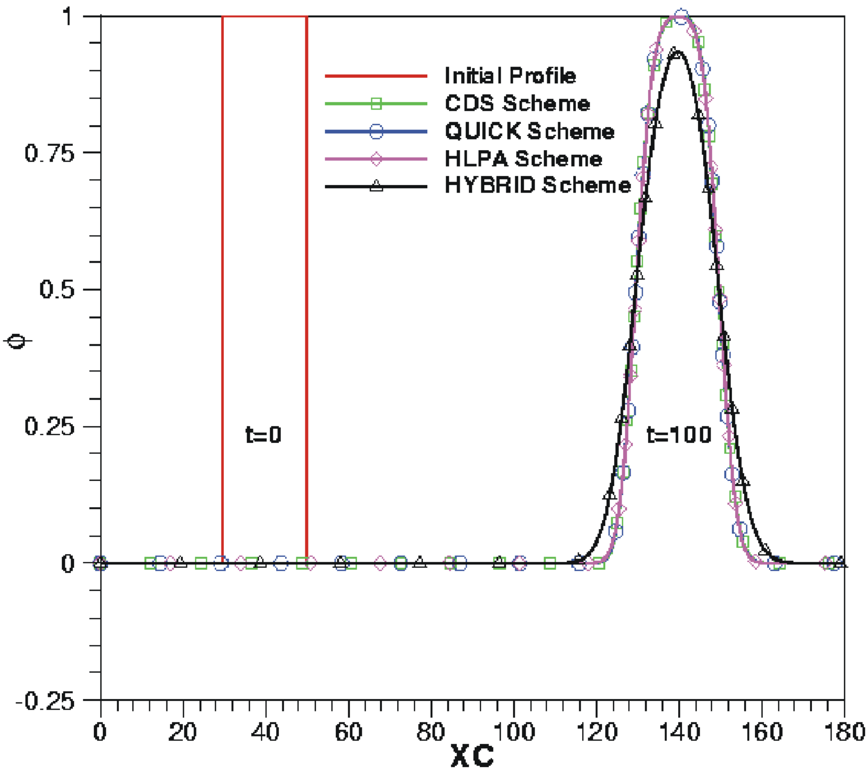


Fig. 3.1 Effect of different spatial discretisation scheme using the 1st order temporal discretisation scheme

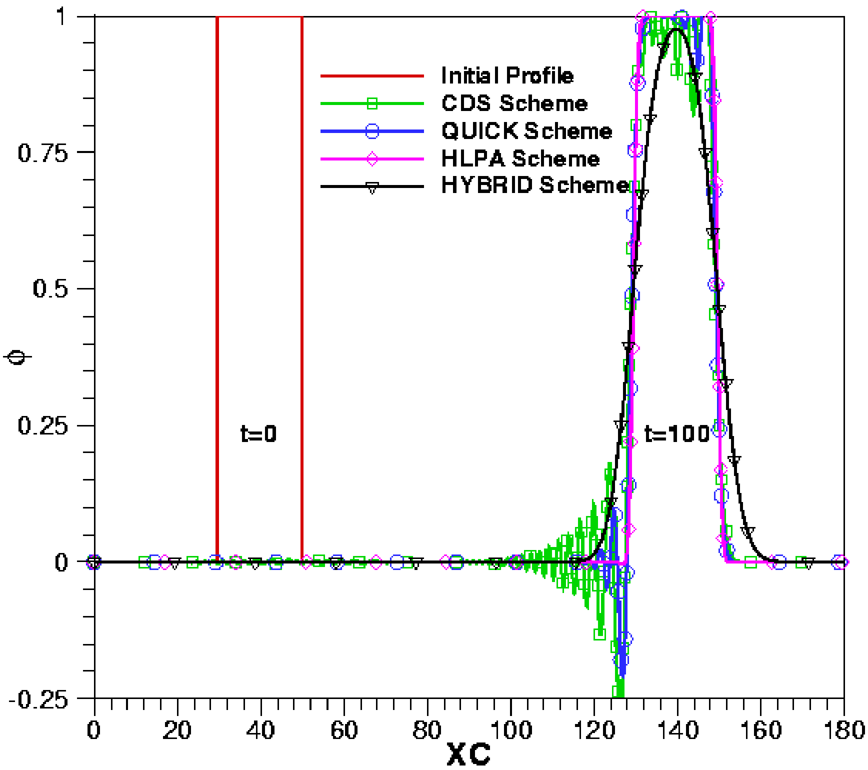


Fig. 3.2 Effect of different spatial discretisation scheme using the 2nd order temporal discretisation scheme

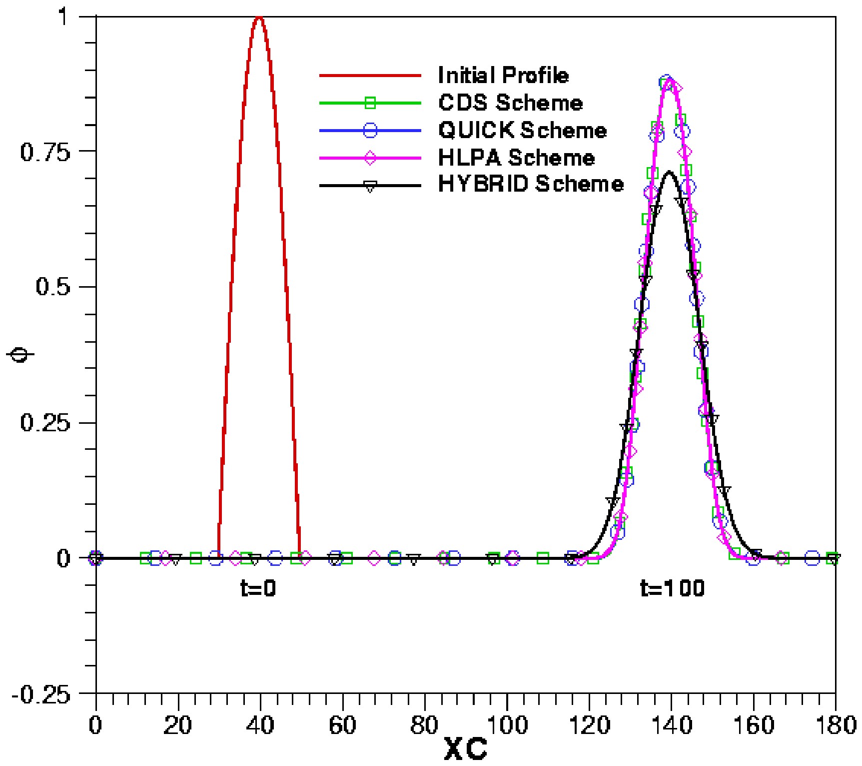


Fig. 3.3 Effect of different spatial discretisation scheme using the 1st order temporal discretisation scheme

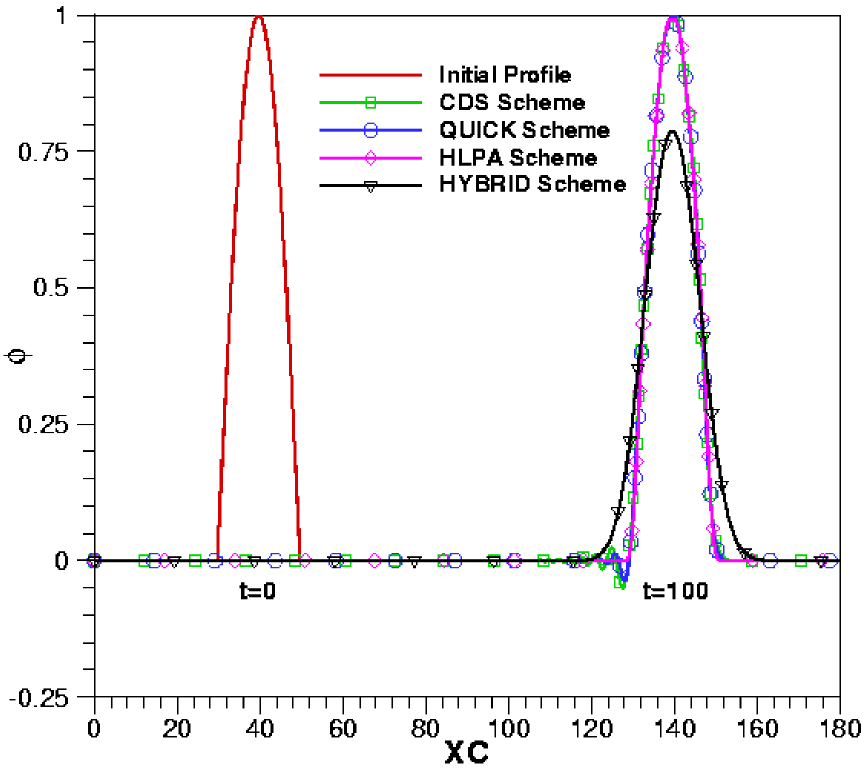


Fig. 3. 4 Effect of different spatial discretisation scheme using the 2nd order temporal discretisation scheme

Fig.3.2 shows the effect of the discretisation scheme on the transport of the same rectangular profile after *t=100* units using the 2nd order accurate temporal scheme and the following observations are made:

- Even using the 2nd order discretisation scheme does not reduce the large numerical diffusion when one uses the Central/Upwind Hybrid discretisation scheme. The rectangular profile is highly diffused to a Gaussian profile with large lateral spread after a few time steps only.
- When the CD and QUICK scheme are used, the sharp rectangular profile is maintained even after t=100 but with some spurious oscillations which are inherent property of these differencing schemes as discussed earlier.
- On the other hand HLPA , as a composite mix between UPWIND and QUICK scheme, limited by the convection boundedness criterion, yields a non-oscillating but sharp rectangular profile even after t=100.

The rectangular profile is simply replaced by a sinusoidal variation at the same x-location in this test case and the initial scalar profile and its location is shown in Fig. 3.3. It is quite evident from the same figure that even for the sinusoidal profile, the numerical diffusion is high when the 1st order temporal discretisation scheme is used, irrespective of the spatial discretisation. However the accuracy is the least and the error is maximum when the Central/Upwind hybrid scheme is used. On the other hand if the 2nd order accurate temporal discretisation scheme is used as shown in Fig. 3.4, the three spatial schemes *viz.*, QUICK, Central Difference and HLPA produce almost the exact solution after t=100, except for some mild oscillations near the profile base specially when the QUICK and Central Difference schemes are used. Even in this case the high numerical diffusion of the HYBRID scheme is quite evident even when the time discretisation errors are small for the 2nd order accurate scheme.

3.2 Two dimensional viscous diffusion of a multiple vortex system

This problem is chosen to test the numerical diffusion effect of the different discretisation schemes in a two dimensional viscous flow situation where the analytical solution is available. This is known as Taylor Problem which analysis the viscous diffusion of a multiple vortex system in a two dimensional field. The analytical solution given below satisfies the continuity and the Navier Stokes equation.

$$\begin{cases} u(x,y,t) = -\cos x \sin y \, \mathrm{e}^{-2t/\mathrm{Re}} \\ v(x,y,t) = \quad \sin x \cos y \, \mathrm{e}^{-2t/\mathrm{Re}} \\ p(x,y,t) = -0.25(\cos 2x + \cos 2y) \, \mathrm{e}^{-4t/\mathrm{Re}} \end{cases} \tag{3.1}$$

$$\text{where } 0 \le x, y \le 2\pi$$

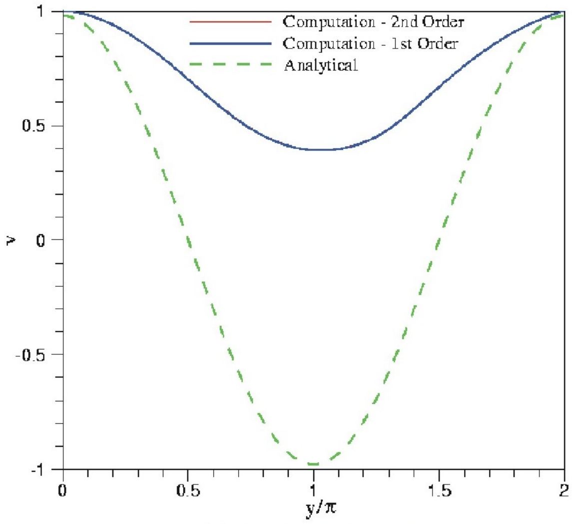
A uniform 62×62 grid is used for a 2D space of length 2π along either direction for a flow Reynolds number Re = 10^4 and the time step size used is Δt = 0.2. The initial conditions of the problem and the boundary conditions at all four boundaries at every time step have been specified using the above equation. All the four spatial discretisation and the two temporal discretisation schemes have been used for numerical solution of the problem. Figs. 3.5 to 3.7 show the comparison between analytical results and numerical computation of *v*-velocity components along *y* direction at $x = 0.48\pi$; *u*- velocity and pressure profiles along x direction at $y=0.48\pi$ respectively and $t= 100$. In this problem too, the figures clearly demonstrate the high numerical diffusion of the Central/Upwind hybrid scheme whereas the agreement is excellent for higher order schemes like QUICK and HLPA. However in this problem the effect of temporal discretisation scheme is observed to be not that significant.

The instanteneous streamlines obtained from analytical solution and the present numerical prediction have been shown in Fig. 3.8. The physical picture of the flow pattern is clearly observed in this figure. The flow consists of multiple vortices with their centre spaced at each π distance along both the x and y directions.

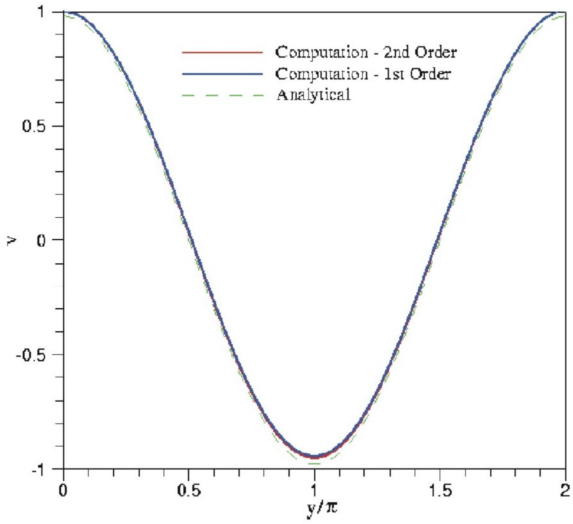
Analytically the vorticity should exponentially decay with time under the action of viscosity showing a change of the flow pattern. Since the Reynolds number chosen is somewhat large, the effect of viscous diffusion is quite small and significant change of the flow pattern is therefore not observed between the results at t=0 and t=100 for the computation with higher order schemes. On the other hand the large numerical diffusion in case of the Hybrid scheme computation has totally changed the flow pattern and the four vortices at the four sides of the domain are observed to be fully mixed with the central vortex. Thus the use of schemes with high numerical diffusion may sometimes lead to a totally wrong physical picture of the flow situation studied.

4. Concluding Reamarks

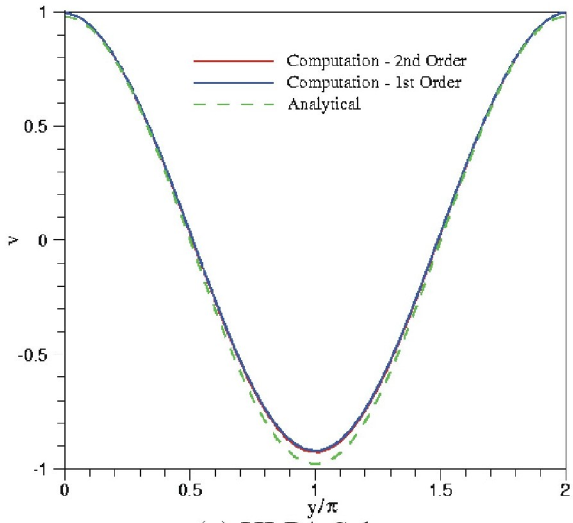
- The numerical diffusion arising out of the truncation error of the spatial and temporal derivative approximation in any discretisation procedure has significant effect on the accuracy of the solution obtained.
- The concept of upwind differencing ensures the numerical stability of any discretisation scheme but at the same time yields very large numerical diffusion leading to unacceptable solution accuracy specially for multidimensional flow problems.
- The higher order schemes like the QUICK or Central Difference schemes or the second order temporal discretisation scheme have the least numerical diffusion but these schemes may sometime yield solutions with non-physical oscillations or serious convergence problem.
- The HLPA scheme, devised through limiting the fluxes by the convection boundedness criterion, is found to be a good compromise between the large numerical diffusion and high numerical instability problems. Most of the CFD algorithms attempt to control the numerical diffusion process, by some means for accurate solution of the flow field. Some algorithms always use central difference scheme and adds artificial dissipation explicitly to enhance numerical stability. Some algorithms use higher order upwind schemes with limitation on fluxes based on some boundedness criterion derived from the neighbouring values of the variable.



(a) HYBRID Scheme

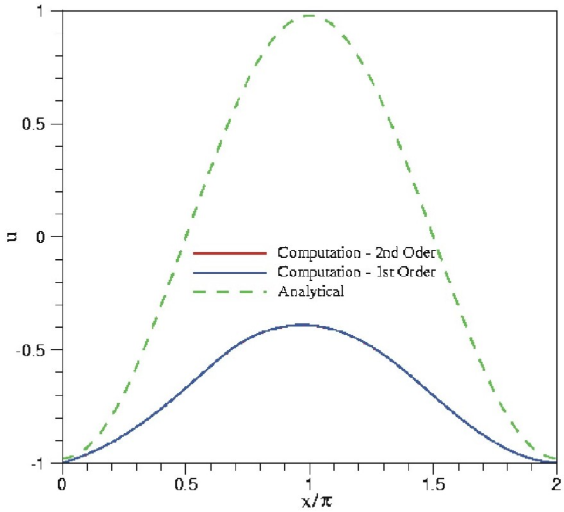


(b) QUICK Scheme

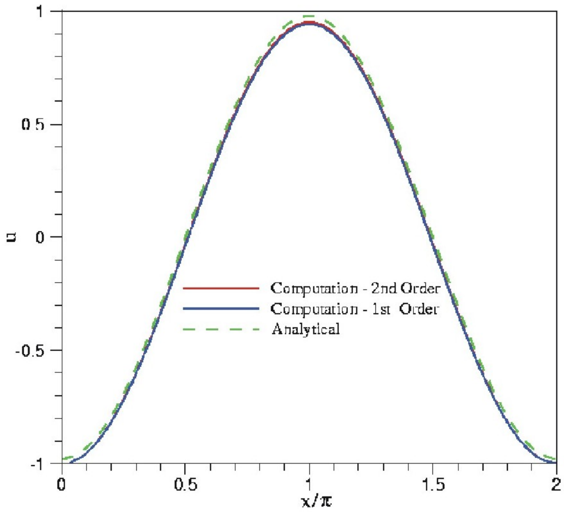


(c) HLPA Scheme

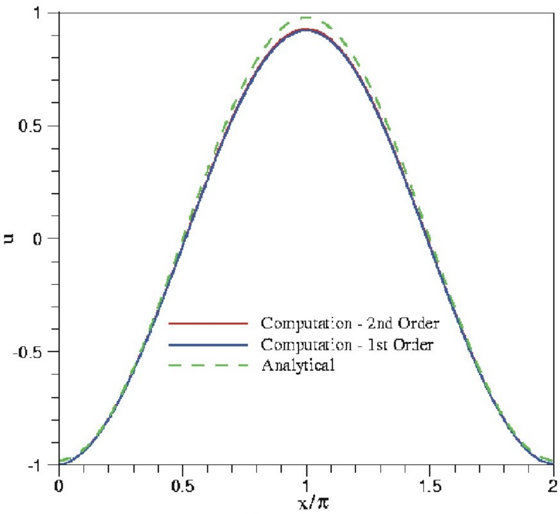
Fig. 3.5 Effect of spatial and temporal discretisation scheme on v-profile at x=0.48π for the Taylor problem



(a) HYBRID Scheme

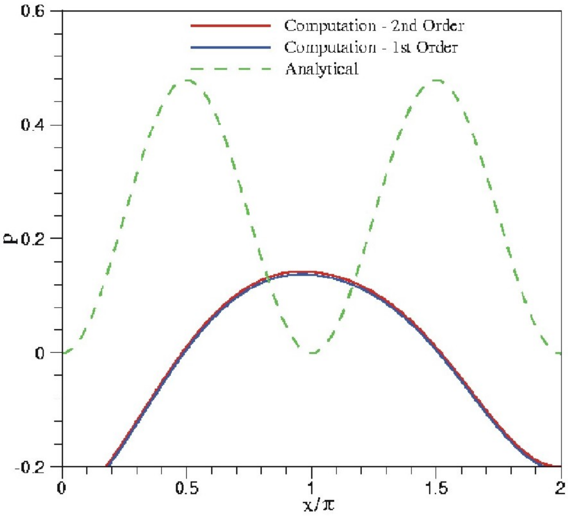


(b) QUICK Scheme

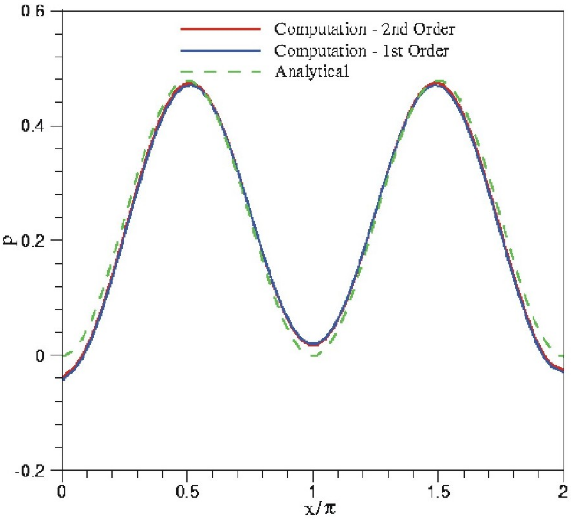


(c) HLPA Scheme

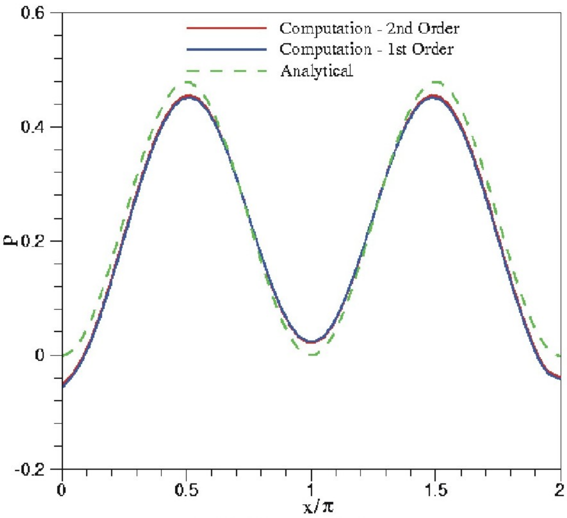
Fig. 3.6 Effect of spatial and temporal discretisation scheme on u-profile at y=0.48π for the Taylor problem



(a) HYBRID Scheme

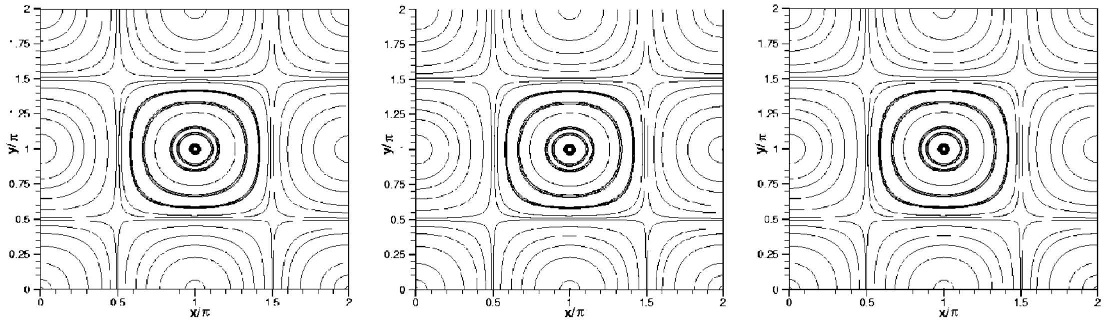


(b) QUICK Scheme



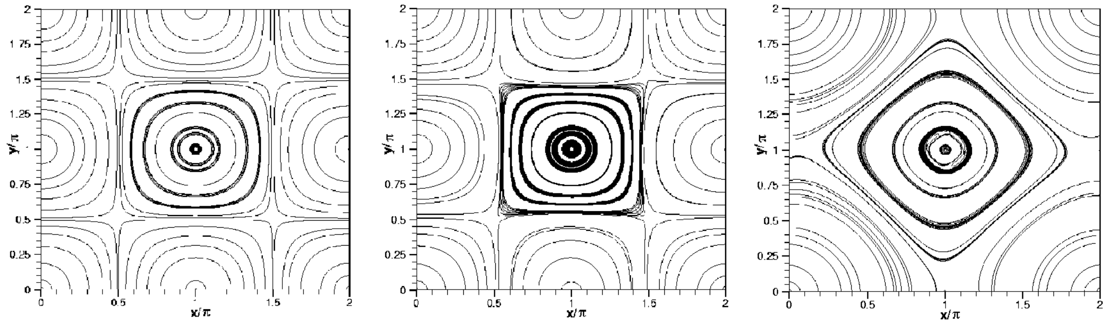
(c) HLPA Scheme

Fig. 3.7 Effect of spatial and temporal discretisation scheme on p-profile at y=0.48π for the Taylor problem



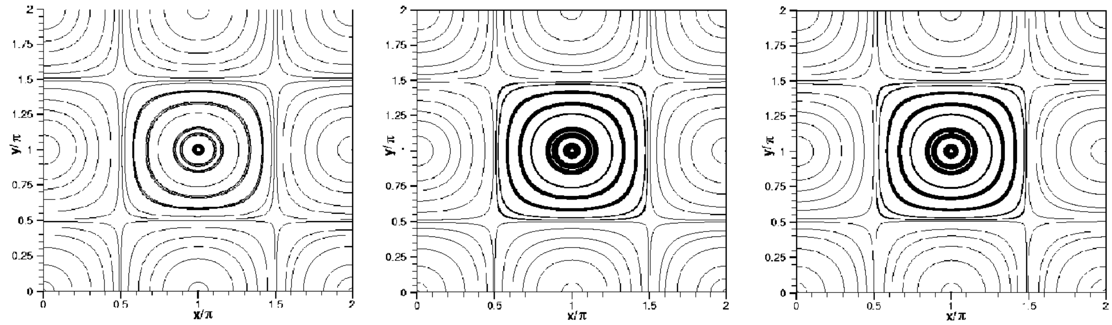
t=0 t=10 t=100

(a) Instantaneous streamlines obtained for the analytical solution



t=0 t=10 t=100

(b) Instantaneous streamlines computed using the HYBRID scheme for spatial discretisation and 2nd order temporal discretisation scheme



t=0 t=10 t=100

(c) Instantaneous streamlines computed using the QUICK scheme for spatial discretisation and 2nd order temporal discretisation scheme

Fig 3.8 Effect of spatial discretisation schemes on the temporal development of the streamlines for the Taylor problem

- The deferred correction procedure is found to be a simple but convenient method of controlling the numerical diffusion through mixing of the fluxes in a desired proportion in order to obtain stable but accurate numerical solution of the flow equations.
- Both the test cases demonstrate stable but accurate and wiggle free solution with second order accurate three level fully implicit scheme for temporal discretisation and HLPA scheme for spatial discretisation

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Studies on the Temporal and Spatial Discretisation Schemes Used in a Pressure-Based RANS Algorithm For Incompressible Flow

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Abstract :

The present work describes the algebra involved in the two different temporal discretisation and four different spatial discretisation schemes implemented in the RANS code RANS3D developed in the CTFD Division for computation of unsteady turbulent incompressible flow in complex configurations. All the schemes are tested on two simple test problems to show the effect of the discretisation schemes on the numerical accuracy of the flow solution.